

Study of the composition of vitamin B6 by IR spectroscopy

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Abstract

In this article, we determined the composition of vitamin B6 using FTIR spectroscopy and using the Carl Zeiss Jena UR-20 spectrometer for wavelengths between 4000 and 400 cm^{-1} . Vitamin B6 (pyridoxine) is an essential water-soluble compound involved in protein metabolism and nervous system function. In this study, the chemical structure of vitamin B6 was investigated by FTIR spectroscopy, in order to identify the characteristic functional groups and to assess the purity of the sample. The FTIR spectrum revealed specific bands corresponding to hydroxyl (-OH), amino (-NH₂) and carbonyl (C=O) groups, confirming the identity and structural integrity of vitamin B6. The analysis demonstrated that FTIR represents a rapid, non-destructive and efficient method for the qualitative characterization of vitamin B6, being useful in the quality control of pharmaceutical products and dietary supplements containing this compound.

Keywords: IR spectrum, vitamin B6, composition

Introduction

Vitamin B6 is one of the B vitamins, and thus an essential nutrient. The term refers to a group of six chemically similar compounds, i.e., "vitamers", which can be interconverted in biological systems. Its active form, pyridoxal 5'-phosphate, serves as a coenzyme in more than 140 enzyme reactions in amino acid, glucose, and lipid metabolism [1,3].

Plants synthesize pyridoxine as a means of protection from the UV-B radiation found in sunlight and for the role it plays in the synthesis of chlorophyll. Animals cannot synthesize any of the various forms of the vitamin, and hence must obtain it via diet, either of plants, or of other animals. There is some absorption of the vitamin produced by intestinal bacteria, but this is not sufficient to meet dietary needs. For adult humans, recommendations from various countries' food regulatory agencies are in the range of 1.0 to 2.0 milligrams (mg) per day. These same agencies also recognize ill effects from intakes that are too high, and so set safe upper limits, ranging from as low as 25 mg/day to as high as 100 mg/day depending on the country. Beef, pork, fowl and fish are generally good sources; dairy, eggs, mollusks and crustaceans also contain vitamin B6, but at lower levels. There is enough in a wide variety of plant foods so that a vegetarian or vegan diet does not put consumers at risk for deficiency. Dietary deficiency is rare. Classic clinical symptoms include rash and inflammation around the mouth and eyes, plus neurological effects that include drowsiness and peripheral neuropathy affecting sensory and motor nerves in the hands and feet. In addition to dietary shortfall, deficiency can be the result of anti-vitamin drugs. There are also rare genetic defects that can trigger vitamin B6 deficiency-dependent epileptic seizures in infants. These are responsive to pyridoxal 5'-phosphate therapy. Vitamin B6 is a water-soluble vitamin, one of the B vitamins. The vitamin actually comprises a group of six chemically related compounds, i.e., vitamers, that all contain a pyridine ring as their core. These are pyridoxine, pyridoxal, pyridoxamine, and their respective phosphorylated derivatives pyridoxine 5'-

phosphate, pyridoxal 5'-phosphate and pyridoxamine 5'-phosphate. Pyridoxal 5'-phosphate has the highest biological activity, but the others are convertible to that form. Vitamin B6 serves as a co-factor in more than 140 cellular reactions, mostly related to amino acid biosynthesis and catabolism, but is also involved in fatty acid biosynthesis and other physiological functions. Because of its chemical stability, pyridoxine hydrochloride is the form most commonly given as vitamin B6 dietary supplement. Absorbed pyridoxine (PN) is converted to pyridoxamine 5'-phosphate (PMP) by the enzyme pyridoxal kinase, with PMP further converted to pyridoxal 5'-phosphate (PLP), the metabolically active form, by the enzymes pyridoxamine-phosphate transaminase or pyridoxine 5'-phosphate oxidase, the latter of which also catalyzes the conversion of pyridoxine 5'-phosphate (PNP) to PLP. Pyridoxine 5'-phosphate oxidase is dependent on flavin mononucleotide (FMN) as a cofactor produced from riboflavin (vitamin B2). For degradation, in a non-reversible reaction, PLP is catabolized to 4-pyridoxic acid, which is excreted in urine [4,17].

Materials and methods

IR spectrum has been recorded in the 400–4000 cm^{-1} spectral range with an UR-20 Carl Zeiss Jena spectrometer, using the pellet technique, with the resolution of 0.6 cm^{-1} .



Fig 1: UR-20 Carl Zeiss Jena spectrometer

Results and discussions

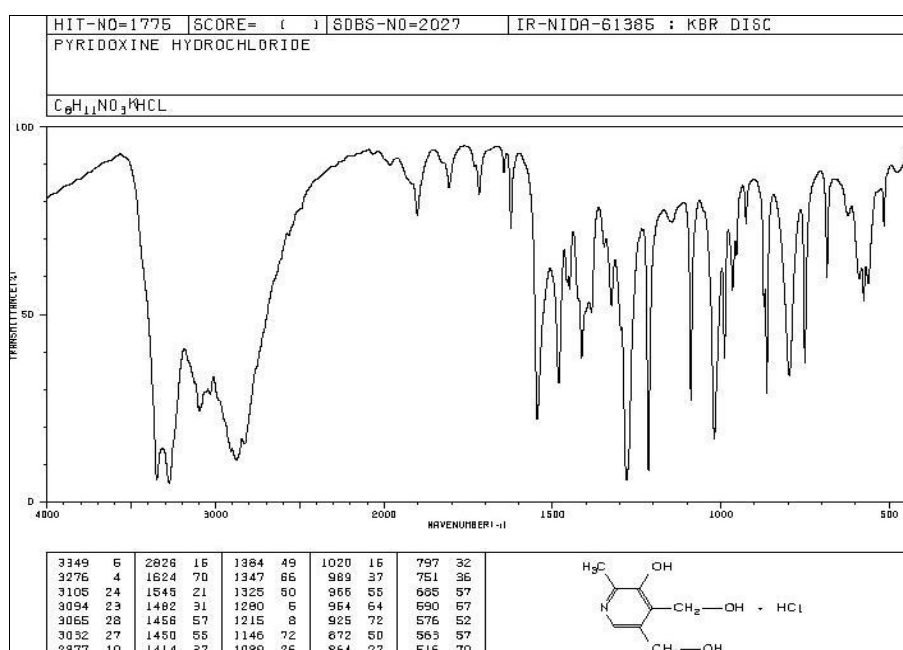


Fig 2: IR spectrum of vitamin B6

Tabelul 1 prezinta alocarea pikurilor pentru vitamina B6.

Table 1: Vibrational data of the B6 vitamin

Band	Vibrational assignment and description
3330 vs	ν (O12-H23).
3284 vs	ν (C11-H21).
3100 vs	ν (C1-H18), ν (N-H).
2880 vs	ν_s (CH3).
2835 vs	ν (C10-H14), ν (C10-H15).
1630 m, 1552 s	δ (H15-C10-H16), δ (C9-N7-H20).
1489 s, 1457 w,	δ (C4-O8-H13), δ (CCO) ν_{as} (CH3), δ (C3-C9-H19).
1400 m	ν (C1-C2, C2-C4) + δ (CH3).
1330 m	δ (C9-N7-H20) + δ (C3-C9-H19) + δ (C-H) + ring tors + δ (H17-C1-O6).
1283 vs	ν (C5-N7) + tors (C5-CH3) + δ (C10-H).
1220 vs	δ (COH); δ (N-H) i.p.
1090 vs, 1023 vs	ring stretch + tors (H17-C1-O6-H24) + ν (CCO).
992 s	δ (N-H) o.p. + δ (C-C) + ν (CCO).
752 vs	tors (H19-C9-N7-H20) + δ (C2-C1-O6) + ν (C1-C2-C3).
687 m, 625 s	tors (C2-C3-C9-H19) + stretch quadrant (C2-C4-C5-N7) + tors (C3-C2-C4-C5)
517 m	δ (OH-C4-C5-CH3) + tors (H19-C9-N7-H20)
477 m	tors (H19-C9-N7-H20) + δ (CCO).

^aAbbreviations: w—weak, m—medium, s—strong, vs—very strong, d—bending, ν stretching, twist—twisting, tors—torsion, i.p.—in plane, o.p.—out of plane.

Conclusions

Vitamin B6 is one of the B vitamins, and thus an essential nutrient. The term refers to a group of six chemically similar compounds, i.e., "vitamers", which can be interconverted in biological systems. Its active form, pyridoxal 5'-phosphate, serves as a coenzyme in more than 140 enzyme reactions in amino acid, glucose, and lipid metabolism. In the FTIR spectrum, absorption bands corresponding to the functional

groups: CH, OH, CH₃, N-H, COO, C-C appear for wavelengths between 4000 and 400cm⁻¹.

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